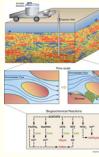


QLBN Sustainable Systems SFA: Evolution of Pore Structures and Flowpath Challenge

QUANTIFICATION OF HYDROGEOLOGICAL CONTROLS AND INDUCED BIOGEOCHEMICAL TRANSFORMATIONS ASSOCIATED WITH IN-SITU BIOREMEDIALTION USING GEOPHYSICAL METHODS

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INTRODUCTION



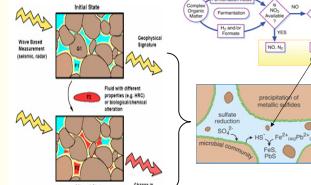
As part of the LBNL SFA 'Evolution of Pore Structure and Flowpath Challenge', we are exploring the utility of geophysical methods for quantifying hydrological controls and induced biogeochemical transformations associated with in-situ bioremediation at the column to local field scales. Our research will help to address a key Evolution Challenge hypothesis that 'the cumulative impact of in-situ remediation-induced transformations will be significant enough to impact flowpaths at the field scale.' Our efforts are focused on the Rifle IFRC site, where bioremediation approaches are being tested within a shallow, unconfined aquifer to immobilize uranium in tailings-contaminated groundwater.

The subsequent poster panels describe the three primary geophysical efforts that are associated with the Evolution Challenge:

PANEL 2: Exploring the geophysical signatures of remediation-induced biogeochemical transformations;

PANEL 3: Developing and testing frameworks that can integrate time-lapse geophysical and geochemical datasets for the estimation of remediation end-products; and

PANEL 4: Quantifying hydrogeological controls and induced biogeochemical transformations at the field scale using our petrophysical insights, estimation frameworks, and time-lapse Rifle datasets.



If informative, the aquifer-scale, geophysically obtained hydrological characterization and biogeochemical monitoring estimates will be used to remotely assess the spatiotemporal distribution of remediation-induced biogeochemical end-products and the control of heterogeneity. This information will be used in turn to parameterize and validate Rifle-based reactive transport models within the 'Evolution of Pore Structure and Flowpath' Challenge.

GEOPHYSICAL SIGNATURES OF BIOGEOCHEMICAL TRANSFORMATIONS

Laboratory Column Experiments

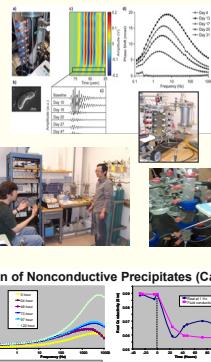
This component focuses on developing an understanding of the geophysical responses of remediation-induced biogeochemical transformations using experimental methods. Previous laboratory-scale research has indicated that seismic attenuation and complex resistivity responses can track the formation of remediation induced FeS precipitates over space and time (e.g., Williams et al., 2005).

However, in order geophysically differentiate between the multiple and often competing processes that occur during biostimulation at the Rifle site, it is necessary to explore geophysical responses to the various potential end-products, such as the complex electrical responses to the evolution of non-conductive precipitates and changes in electroactive ion composition.

Geophysical Responses to the Evolution of Nonconductive Precipitates (Calcites)

Precipitation of non-conductive calcite was abiotically induced through by introducing Na₂CO₃ to CaCl₂ saturated Rifle sediments in a flow through column (calcium, 33 mM; carbonate, 33 mM). The experiment is in progress with current observations:

1. Calcite precipitation causes significant decrease of fluid conductivity and column electrical conductivity
2. An increase in phase and imaginary conductivity is observed at high frequencies and late time, synchronous with visible onset of calcite precipitation.
3. Calcite precipitation promotes polarization behavior of natural sediments due to the small grain size and increase in surface area.



Geophysical Responses to Changes in Electroactive Ion Composition (e.g., Fe(II) and bisulfide)

Laboratory column experiments were performed to explore the complex electrical response to changes in electroactive ion composition accompanying acetate amendment of U(IV) and Zn(II) biostimulated CO₂ sediments. Increases in both the electrical conductivity and polarization terms accompanied both stimulated iron and sulfate reduction, with the changes in both terms increasing according to the accumulation of both electroactive ions and sulfide minerals.

These experiments show that the complex electrical signature responds to both the evolution of different precipitates and changes in electroactive ion composition. Subsequent experiments will explore the geophysical responses to multiple and sequential evolution of different end-products within the same column.

Reference: K.H. Williams et al., Geophysical monitoring of microbial activity during stimulated subsurface bioremediation, submitted to *Environ. Sci. Technol.*, 2009.

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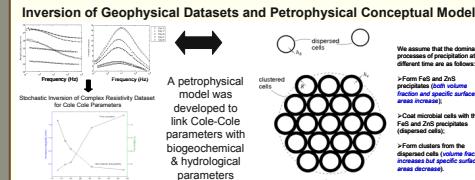
BIOGEOPHYSICAL ESTIMATION FRAMEWORK

Bayesian Frameworks

In order to use the time-lapse geophysical data to quantitatively estimate biogeochemical end-products, it is necessary to develop a framework that can integrate time-lapse geophysical, geochemical, and other types of datasets with petrophysical relationships in the estimation of biogeochemical parameters. To meet this objective, we have developed a state-space Bayesian approach that uses Markov Chain Monte Carlo sampling methods to find the solutions. This model requires estimates of Cole-Cole parameters (inverted from complex resistivity data) and a petrophysical model to link the geophysically-obtained estimates with the biogeochemical properties.

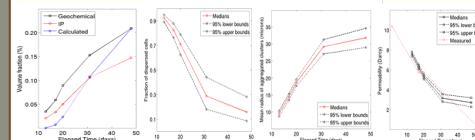
$$\begin{aligned} & f(p_1, p_2, \dots, p_n | x_1, x_2, \dots, x_n, d_1, d_2, \dots, d_n) = \\ & \propto f(x_1 | p_1, d_1) \times f(x_2 | p_2, d_2) \times \dots \times f(x_n | p_n, d_n) \quad \text{Prior information} \\ & \times \exp\left(\frac{1}{2\sigma^2} \sum_{i=1}^n \left(\frac{x_i - G(p_i, d_i)}{\sigma}\right)^2\right) \quad \text{Geophysical data} \\ & \times \exp\left(\frac{1}{2\sigma^2} \sum_{i=1}^n \left(\frac{p_i - G(p_i, d_i)}{\sigma}\right)^2\right) \quad \text{Normalized geobio} \end{aligned}$$

Time constant



Framework Testing using Column Datasets

We have applied the framework to the complex resistivity data collected during column experiments designed to precipitate FeS and ZnS during biostimulated-induced sulfate reduction (Williams et al., 2005) to estimate the evolution of: volume fraction of isolated precipitates (left), fraction of the dispersed, sulfide-encrusted cells (middle left); mean radius of aggregated clusters (middle right), and associated permeability over the course of the experiment due to pore clogging by the precipitates (right).



Our results suggest the developed state-space approach permits the use of geophysical datasets for providing quantitative estimates of the evolution of end-products and permeability reduction associated with biogeochemical transformations at the column scale. Efforts are underway to enable application of the framework to spatially-distributed field datasets.

References

- Chen, J., A. Kemna and S. Hubbard, A comparison between Gauss-Newton and Markov-chain Monte Carlo-based methods for inverting spectral induced-polarization data for Cole-Cole parameters, *Geophysics*, 73(2), F247-F259, DOI 10.1190/1.2976115, 2008.
 Chen, J., Susan S. Hubbard, Kenneth H. Williams, Steve Pride, Li Li, and Lee Slater, A state-space Bayesian framework for estimating biogeochemical transformations using time-lapse geophysical data, submitted to *WRR* 2009.

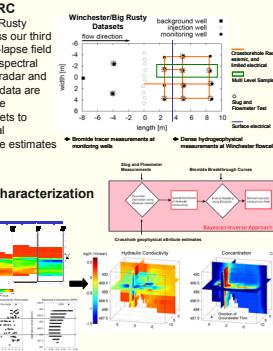
FIELD-SCALE HYDROGEOPHYSICAL CHARACTERIZATION AND BIOGEOPHYSICAL MONITORING

Data Acquisition at the Rifle IFRC

In collaboration with the Rifle IFRC Big Rusty biostimulation experiment and to address our third objective, we have collected a rich time-lapse field geophysical dataset, including: surface spectral induced polarization data, tomographic radar and seismic data, and wellbore logs. These data are being used together with time-lapse Rifle hydrogeological and geochemical datasets to estimate in-situ baseline hydrogeological heterogeneity and to provide quantitative estimates of remediation-induced biogeochemical transformations.

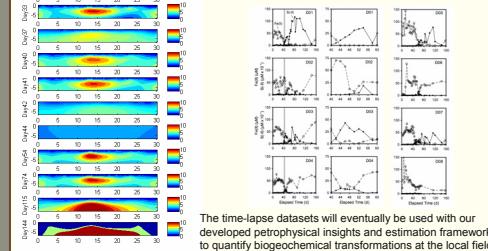
Rifle IFRC Hydrogeophysical Characterization

A Bayesian-Inverse approach has been developed that can incorporate wellbore, tracer, and tomographic data in the holistic estimation of hydraulic conductivity. The method has been tested using Rifle-based datasets and is being refined to account for complex injection and dynamic gradient functions.



Rifle IFRC Biogeophysical Monitoring

Preliminary analysis of the spectral induced polarization data (left) and comparison with time-lapse wellbore geochemical data collected during biostimulation at the Rifle site (below) indicates sensitivity to spatiotemporal changes in electroactive ion concentration and the accumulation of semi-conductive mineral precipitates.



The time-lapse datasets will eventually be used with our developed petrophysical insights and estimation framework to quantify biogeochemical transformations at the local field scale.

Reference

- Englert, A., M.B. Kowalsky, K. Williams, J. Peterson, F. Spane, D. Newcomer, P. Long and S. Hubbard, Estimation of a three dimensional hydraulic conductivity field at the Rifle, CO Integrated Field Challenge Site using a Sequential Bayesian-Inverse Approach, CMWR XVII, San Francisco, July 7-10, 2008.